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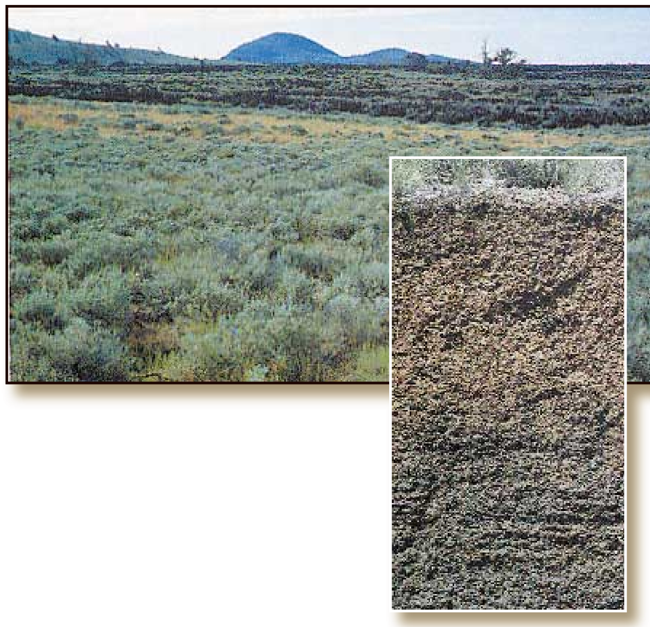
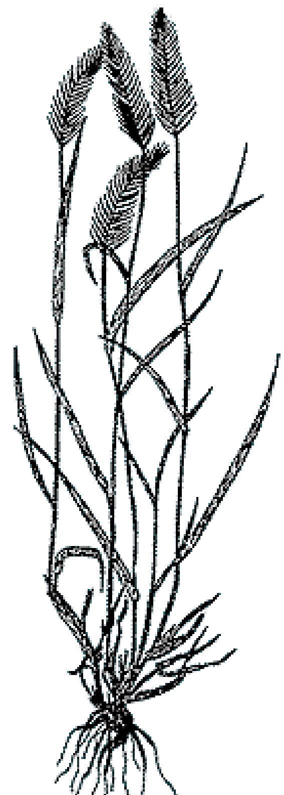
In This Issue





Understanding the Biogeochemistry of Cesium

—An Investigation of Factors Influencing Cesium Mobility

It is impossible to understand the factors affecting cesium's fate in soil without examining the system of soil/plant/microbe interactions. The INEEL is leading a systematic and collaborative research effort to not only understand the complex interactions of this system, but also to develop a mathematical model.

Cesium is one of the Department of Energy's (DOE's) most common and recalcitrant soil contaminants. It binds strongly to soil components, making it difficult to remediate. However, plants are capable of concentrating it in their tissues, a process called bioaccumulation. This fact may be the key to unlocking cesium's mobility in soil.

> *"We decided to use a systems engineering approach to develop our conceptual model."*
>
> — M. Hamilton, INEEL biotech manager

A multi-institutional research team is examining how cesium mobility is affected by geochemical interactions with clay minerals, soil microbes, and exudates, which are substances produced by plant roots. The team's working hypothesis is that cesium is tightly bound in the sheet structure of clay minerals, but its interaction with organic compounds (e.g., plant and microbial exudates) increases its bioavailability through biogeochemical alteration. Understanding the interactions will both improve the DOE's prospects for predictive modeling and

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enhance field activities, ranging from improved remediation and risk reduction choices to better cap designs.

To understand how cesium is partitioned among the soil, water, and plant phases, the team decided to model the factors and inter-relationships affecting cesium mobility as an ecological unit. "We decided to use a systems engineering approach to develop our conceptual model," said Melinda Hamilton, INEEL biotech manager and the project's original principal investigator. "The conceptual work gave us a firm foundation for designing experiments and formed the basis for our mathematical models."

The conceptual model (see Figure 1) categorized the processes affecting cesium mobility into six sub-models: geochemistry, physical factors, root system density, microorganisms, nutrients, and root exudates. A seventh sub-model (cesium fate) describes cesium movement among the soil, water, and plant phases.

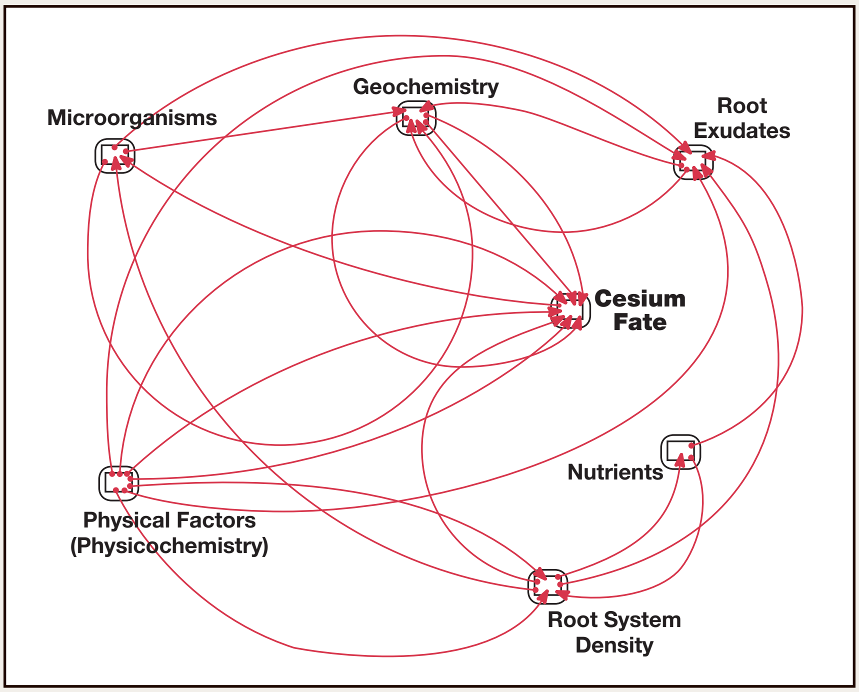

Figure 1. A simplified illustration of the conceptual model of cesium mobility in soil.

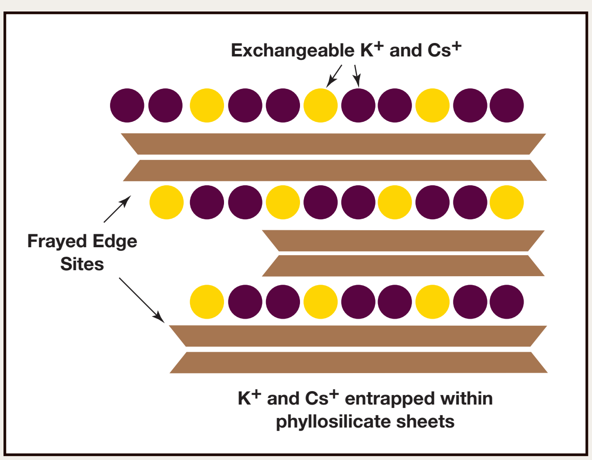

Figure 2. The sheet structure of micaceous clay minerals, such as illite and smectite, can entrap both cesium and potassium.

Experimentation to expand and quantify the six sub-models is being carried out by a variety of institutions and disciplines. Paul Bertsch, director of the University of Georgia's Savannah River Ecology Laboratory (SREL), has examined how cesium is bound in soils. Bertsch and his colleagues characterized mineral and organic constituents in samples collected from the INEEL and elsewhere to identify cesium's associations with reactive mineral phases.

Their research confirmed the suspicion that the cesium is trapped in the sheet structure of micaceous clay minerals, primarily illite and smectite. These minerals, particularly illite, appear to control cesium's sorption.

Bertsch, one of the foremost experts on the interaction of contaminants and clay mineralogy, suspected that the frayed edge sites of these minerals (see Figure 2) are critical to understanding the sorption and desorption of cesium. He developed a new method for quantifying the number of frayed edge sites in soils. The technique allows sorption at frayed edge sites to be correlated with other factors suspected to contribute to cesium mobility, such as interaction with root exudates.

Roots exude substances that are important in the function of the plant/soil system. The exudates are typically low molecular weight compounds such as sugars, phenols, and organic and amino acids that are produced and transported by plants to the soil in the root zone. The team suspects that cesium's bioavailability is increased by the interaction of exudates with clay minerals, but there is a lack of information about which exudates are important and why.

Bruce Bugbee, director of the Utah State University (USU) Crop Physiology Laboratory, has developed a new laboratory method to recover, isolate, identify, and quantify specific root exudates. This technique was applied in the first set of experiments (see Figure 3).

Since root exudates can vary with the type and amount of plant stress, the next experiments will stress plant systems in various ways so the resulting exudates can be examined. Potassium and cesium, both alkali metals, are essentially chemically interchangeable in the way they bind with clay minerals, so exudates resulting from potassium stress are of particular interest.

> ***"We would like to know which exudates have the greatest influence on cesium uptake, and therefore, cesium mobility."***
>
> *— C. Palmer, INEEL geochemist and principal investigator*

"We would like to know which exudates have the greatest influence on cesium uptake, and therefore, cesium mobility," said Carl Palmer, an INEEL geochemist and the project's current principal investigator. "The next step is to take what we've learned from the work at SREL and USU and look at the chemical mechanisms."

Laura Hanson, a graduate student from Washington State University (WSU), is working with Palmer at the INEEL to confirm the chemical effects of root exudates on clay minerals. "We suspect that root exudates are chemically weathering the edges of clay minerals, which release the cesium and potassium for plant uptake," said Hanson, who is working on a Ph.D. dissertation examining how cesium is bound to and released from soils.

In addition to root exudates, microbes also play a complex role in cesium bioavailability. Some microbes cause plants to increase exudate production. Other microbes metabolize exudates as a source of energy, thereby removing them from the system. Microbes may also produce their own exudates. As a result, they can either enhance or retard the effects of root exudates in liberating cesium.

Figure 3. USU researchers are growing Hycrest crested wheatgrass** (Agropyron cristatum X Agropyron desertorum) **in sterile hydroponic systems to create controlled root-zone environments from which exudates can be isolated.
(photo courtesy of USU Crop Physiology Laboratory)

To understand these complex interactions, INEEL microbiologist Tom Ward will collaborate with USU to introduce microbes to their hydroponic experiments with crested wheatgrass. Ward is also examining how, or whether, microbial interactions affect the structure of clay minerals, such as illite and smectite.

The sheet structures of these minerals, which researchers suspect entrap the cesium, are held together partly by the bonding of aluminum. "The lattice structure of these minerals may be weakened by compounds that chelate aluminum," said Ward. "If so, microbes that secrete compounds that effectively chelate aluminum should have an effect on the mobility of cesium."

To test this hypothesis, Ward has been modifying an established assay for detecting iron chelators to permit aluminum chelating compounds to be detected. "Once the assay is refined so that we know we are isolating bacterial colonies that secrete compounds that chelate aluminum, we will be able to test the effect these microbes have on cesium partitioning in the soil phase," said Ward.

> ***"We hope to create an integrated model that is predictive and incorporates the complex biogeochemistry we are beginning to understand."***
>
> *— Carl Palmer, INEEL geochemist and principal investigator*

The results of Ward's research and the other investigations will be used to fill in the conceptual model. "We hope to create an integrated model that is predictive and incorporates the complex biogeochemistry we are beginning to understand," said Palmer.

Lori Siegel, a Northeastern University graduate student, will build a mathematical construct based on the INEEL's research and other information for her Ph.D. dissertation. She plans to incorporate the functional relationships and parametric values in and between the sub-models of the conceptual model to more fully describe the interaction of

(Cesium continued on page 4)

(Cesium continued from page 3)

root exudates in cesium partitioning. No model like this has previously been developed.

Once constructed, the model will be validated through further experiments and field testing. The INEEL Engineered Barrier Test Facility, a mesoscale facility, may be used for the field tests because it offers access to larger-scale experimental plots with greater control of conditions. In addition, testing the newly developed model at this facility would provide data on performance of vegetative and engineered caps.

Having a better understanding of cesium partitioning among soil, water, and plant phases is expected to have broad benefits to DOE. Phytoremediation techniques, which use plants to take up and concentrate cesium, can be improved. On the other hand, techniques that retard cesium uptake could also be beneficial, particularly in areas where range fires can potentially release bioaccumulated cesium.

"Even though this is basic research, we are always considering the many ways we can use what we've learned," said Palmer. "Thinking about ways to integrate and apply our results is part of the INEEL culture."

Note: This research is funded by the Environmental Systems Research Candidate program and is being conducted by: Carl Palmer, Ph.D.; Melinda Hamilton, Ph.D.; and Tom Ward, Ph.D. (all from the INEEL); in collaboration with Bruce Bugbee, Ph.D. (USU); Paul Bertsch, Ph.D. (U. of Georgia); Laura Hanson, (WSU); and Lori Siegel (Northeastern U.).

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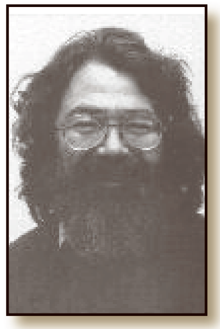
New Staff Add Capabilities in Modeling and 4-D Geophysics

Meakin Joins as Fellow



Paul Meakin

Paul Meakin didn't know the Subsurface Science Initiative (SSI) existed until he discovered its Web site. At the time, he was in Norway, pursuing research as a professor at the University of Oslo. Meakin was familiar with the lab's location, having vacationed in the region, and the SSI piqued his interest. So he submitted his credentials.

Meakin joined the SSI as a Scientific Fellow in November 2001. His primary research objective is to form a modeling group skilled in interpreting the subsurface environment and to pursue research in subsurface pattern formation, fluid flow in both fractured and porous media, fractals, geomorphology, and the growth of rough surfaces.

"Joining the Initiative at this stage provides a great opportunity to have an influence on the research direction at the INEEL," said Meakin. He also plans to take advantage of the area's varied outdoor recreation opportunities.

Meakin earned his B.S. in chemistry from the University of Manchester in Great Britain, and completed a Ph.D. in physical chemistry at the University of California, Santa Barbara, in 1969. After graduation, he accepted a post-doctoral position with the DuPont Company, where he remained for 23 years as a researcher and research program manager. Meakin's research included homogeneous catalysis, nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) spectroscopy, superionic conductivity, atmospheric science (modeling the effects of freons on ozone depletion), polymeric liquid crystals, and ion exchange membranes. He also pursued an interest in statistical physics and fractal geometry.

In 1991, Meakin left DuPont and joined the University of Oslo Department of Physics. While there, he was involved in a joint physics/geology strategic university program on fluid/rock interactions. His work also included multiphase flow in porous media, computer modeling of meandering river channels, and corrosion and fracture processes.

> ***"Joining the Initiative at this stage provides a great opportunity to have an influence on the direction of the research at the INEEL."***
>
> *— P. Meakin, INEEL SSI fellow*

SSI director Mike Wright thinks Meakin will make substantial contributions to the INEEL subsurface science research community. "The breadth of Paul's experience continues to amaze me. When he is in a seminar, his questions drive straight to the fundamental core of the topic. His inquiries trigger the types of discussions you hope for when you are a serious researcher, and Paul always has highly relevant research experience in his background that gives him that insight," said Wright.

Meakin will be focusing on three primary areas at the INEEL, including:

- Fluid flow in fractures—examining a wide range of partially saturated conditions from high infiltration regimes to thin films in nearly desiccated conditions,

- Colloid behavior and control—determining what controls can be exercised to 1) direct, restrain, or block flow, 2) deliver nutrients, or 3) use the sensitivity of colloids to their physical environment as tracers or indicators of subsurface conditions,
- Mineral dissolution in subsurface systems—particularly focussing on how creation of surface roughness has consequences for chemical and biotic behavior in both wet and dry conditions.

Meakin is a fellow in the American Physical Society and a member of the Norwegian Academy of Science and Letters. He has more than 290 refereed publications to his credit, and 60 other publications. His book *Fractals, Scaling and Growth Far From Equilibrium* was published in 1998 by Cambridge University Press.

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Versteeg Joins Geophysics Characterization Team


Roelof Jan Versteeg

Roelof Jan Versteeg decided to join the INEEL's SSI team after a recent meeting with SSI geophysics discipline lead Russ Hertzog at the 2001 Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Hertzog is enthusiastic about Versteeg's interest and background in the automation of geophysical data collection and processing. "We are really lucky to have him join our team," said Hertzog. "Roelof is very respected for his work in near-surface geophysics. He is clearly a leader who knows how to build programs and advanced research capabilities."

Prior to accepting the position, Versteeg created and led the Environmental and Engineering Geophysics (EEG) program at Columbia University and its associated research facilities at the Lamont Doherty Earth Observatory.

Versteeg is particularly experienced in applying repeated geophysical surveys—4-D geophysics—to observe the migration or change of a contaminant in the near surface. He has focused on noninvasive, nondestructive examination of alterations (e.g., contaminant migration) in subsurface conditions, using geophysical techniques such as Ground Penetrating Radar (GPR) and electrical resistivity.

> **" I think that to really solve the problem of process imaging, geophysical observations should be coupled to hydrological modeling, geochemistry, and direct characterization."**
>
> *— R. Versteeg, INEEL SSI geophysicist*

"I think that to really solve the problem of process imaging, geophysical observations should be coupled to hydrological modeling, geochemistry, and direct characterization," said Versteeg. "That's the exact direction INEEL is following, and I am very excited and happy to be a part of it."

Versteeg earned a B.S. and M.S. in geophysics, as well as an M.S. in geology, from Utrecht University in the Netherlands. He received a Ph.D. in geophysics from the University of Paris VII in 1991, followed by a post-doctoral position at the Institut Francais du Petrole in Rueil Malmaison, France. Then, as a visiting scientist at Amoco Production and Research Laboratory in Tulsa, Okla., he worked on pre-stack depth migration methods. This was followed by a period as a research scientist in the Department of Computational and Applied Mathematics at Rice University, where he developed seismic inversion methods with emphasis on integrating geological constraints.

Prior to leading Columbia's EEG program, Versteeg initiated a near-surface and environmental geophysics program at the University of Connecticut. He was also a member of New York City's committee for brownfields restoration.

Versteeg is a member of the American Geophysical Union, Society of Exploration Geophysics, European Association of Exploration Geophysics, International Association of Sedimentologists, and the Environmental and Engineering Geophysical Society. He has edited numerous books, journals, and proceedings in his field, including work for *Geophysics* and the *Journal of Environmental and Engineering Geophysics*. He has authored or co-authored more than 20 peer-reviewed publications and numerous conference proceedings.

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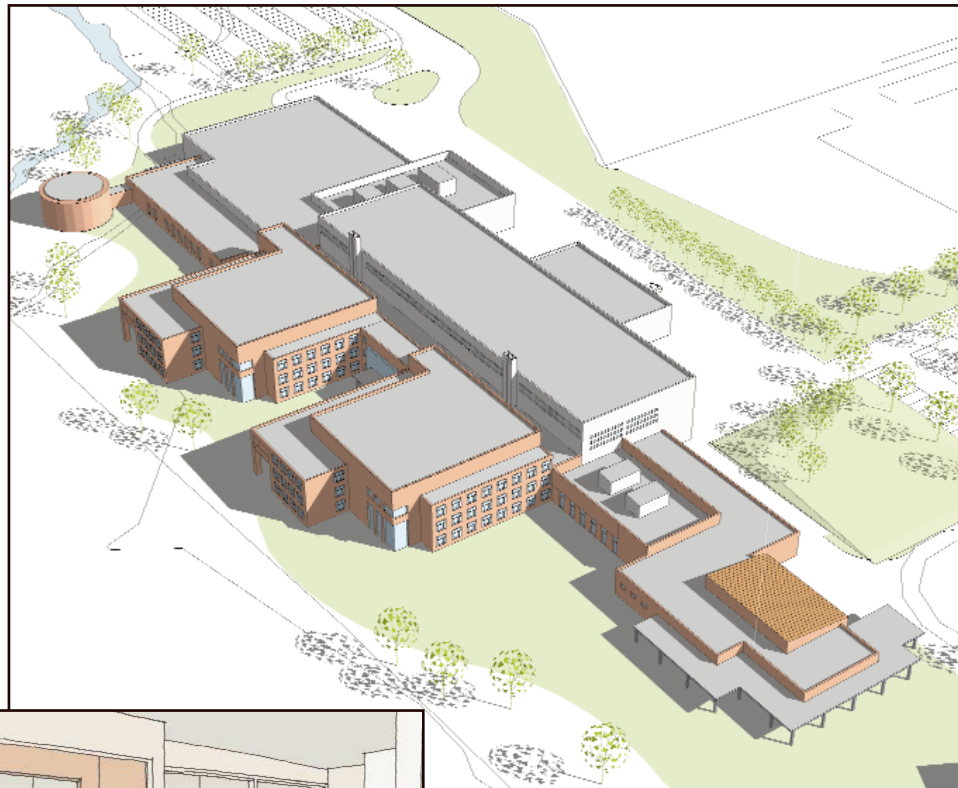
SGL Conceptual Design Phase Nearing Completion

—Report to be Issued

INEEL staff members are finalizing the cost estimates for the INEEL's Subsurface Geosciences Laboratory (SGL) and finishing the Conceptual Design Report. They plan to submit the report to DOE for approval this spring. The report is based on the conceptual design vision delivered to the INEEL by the Zimmer-Gunsul-Frasca Partnership (ZGF) architectural and engineering firm in January 2002.



Crafting facility design to suit research needs

Conceptual design is the first of three phases in the project to build the SGL facility. It requires an intensive collaborative effort between the researchers, who define the working requirements for the facility, and the architectural and engineering design team, which converts those needs into a visual, working concept. Building renderings, floor plans, and the location and size of key functional areas are identified in this phase.

> ***" This phase provides us with the details we need to establish preliminary project baselines, including scope, schedule, and budget."***
>
> *— W. Ridgway, INEEL SGL project manager*

"The conceptual design phase is crucial for identifying the issues and risks associated with the project while turning the technical requirements identified by the researchers into practical building designs," said Wayne Ridgway, INEEL's project manager for the proposed SGL facility. "This phase provides us with the details we need to establish preliminary project baselines, including scope, schedule, and budget."

Ridgway's responsibilities include making sure the design team and the researchers who will use the laboratory are 'on the same page' so that the researchers' technical requirements are fulfilled. The facility design, for example, needs to segregate stray electromagnetic signals from some of the experimental areas, and the proposed 5.5-meter geocentrifuge must be isolated from vibrations generated in other parts of the facility. At the same time, the environment must be conducive to collaboration among researchers.

> ***" Clearly, the SGL will have the functionality we need for conducting large-scale experiments to help solve DOE's cleanup problems."***
>
> *— Mike Wright, INEEL SSI director*

ZGF translated these and many other requirements into building designs, floor plans, and renderings, which were then repeatedly evaluated by the scientists.

"It is vitally important that the research scientists who will use the laboratory have an opportunity to work closely with the engineers and architects doing the design work. This is especially true with a facility as unique as the SGL," said SSI Director Michael Wright. "I am very pleased with the design team's interaction with our research group. Clearly, the SGL will have the functionality we need for conducting large-scale experiments to help solve DOE's subsurface cleanup problems."

What's next?

The delivery of the Conceptual Design Report marks the end of the conceptual design phase. The information in the report is used to gain approval—a step known as Critical Decision 1—to proceed to the next phase, the preliminary design phase.

> ***" We have approximately two more years of design work before we will be ready to begin construction."***
>
> *— W. Ridgway, INEEL project manager*

Preliminary design (previously called Title I design) finalizes alternatives and is used as the basis for the construction budget request. Final design (previously Title II design) is the third and last phase. It provides the details necessary to construct the facility.

"We have approximately two more years of design work before we will be ready to begin construction," Ridgway said. "But with conceptual design nearly wrapped up, we know our proposed facility meets the research requirements and we have the detail necessary to provide an accurate cost estimate. From a project management perspective, we are on track."

Challenges ahead

The current operating environment may pose some stiff challenges for obtaining approval and funding for the next step of design. The new administration in Washington, D.C. is re-examining the need for proposed DOE facilities, even those already in the conceptual design phase at the time of the transition. In addition, a major reorganization is under way in DOE's Environmental Management office.

The INEEL plans to forge ahead with the SGL despite these issues. "We knew from the start that the 2000 presidential election would result in a discussion of our research and facility needs with new DOE management," said Wright. "But we feel very strongly that DOE needs the research capabilities we're proposing if it is to meet its environmental mission objectives."

Meanwhile, the design work continues. "We have worked very closely with the researchers, iterating designs and double-checking crucial aspects of facility design and performance," said Ridgway. "Now, our job is to take the requirements document, turn it into a conceptual design for a facility, and then establish the level of resources required to complete the project. We are almost there."

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Troubleshooting Prompts Discovery

The microbes that have been plugging up extraction wells at the INEEL may one day be used to remediate the primary contaminant in those wells—carbon tetrachloride. An INEEL scientist isolated the microbes while investigating how the wells, used to remove organic vapors from the vadose zone, were getting fouled.

The wells are part of a vapor vacuum extraction system that has been operating since 1996 (see sidebar on next page). Recently, however, two of the six extraction wells became plugged. A video log of a well casing showed a grayish-brown viscous material oozing from the slots in the screened intervals—evidence of microbial activity. The INEEL biotechnology group was called in to identify the culprit and find solutions for the problem.

> ***" I wanted to see if the microbial community we cultured was capable of dechlorinating carbon tetrachloride."***
>
> *— B. Lee, INEEL microbiologist*

Identifying the suspects

Microbiologist Brady Lee began by culturing a sample of the material. Through a series of enrichment processes, Lee produced a microbe population that included iron-reducing bacteria. The enrichment process itself produced a significant amount of an extracellular polymer capable of clogging the wells.

Based on the results of the enrichment processes and other tests, Lee concluded that the most likely cause of well fouling was extracellular polymer produced by microbes involved

(Discovery continued on page 8)

(Discovery continued from page 7)

in iron cycling in natural environments. When the screened interval of the well became saturated with water from infiltration or condensation, microbes from the screening materials and the surrounding geological media proliferated, producing the material that is probably responsible for plugging the wells.

Additional experiments revealed that the silica sand, bentonite clay, and crushed basalt used to construct the screened interval of the well not only furnished a source of microbially reducible iron but also, possibly, the microbes themselves.

Bentonite is possibly the biggest culprit. It contributes more microbially reducible iron than the other materials, which results in more bacterial growth and production of extracellular material. The material also appears to polymerize with dissolved bentonite, producing the grayish-brown viscous material observed in the video log.

Lee's understanding of how the wells were biofouled gave remediation managers the information they needed to make cost-effective decisions about solving the problem. Controlling future problems may be as simple as using anti-microbial compounds to inhibit microbial growth in the packing material.

But the iron-reducing microbes aroused Lee's curiosity. "Since the extraction wells are used in a system for removing chlorinated solvents, especially carbon tetrachloride, I wanted to see if the microbial community we cultured was capable of dechlorinating carbon tetrachloride," Lee said.

Pursuing the possibilities

The results of his next experiments confirmed that dechlorination was occurring. Under aerobic conditions, the microbial community began to grow, quickly removing the oxygen. Dechlorination of the carbon tetrachloride appeared to begin when the oxygen was removed. This was evidenced by a decrease in carbon tetrachloride and a substantial increase in chloroform in the cultures. The bacterial growth occurred with Fe (III) ethylene diamine tetra-acetic acid (EDTA) as the electron acceptor, and with insoluble sources of ferric iron, such as silica sand, crushed basalt, and bentonite.

The growth medium in the enrichment vials was initially yellow, but began to clear, indicating the reduction of iron. A gelatinous substance (the likely cause of well fouling) formed in vials for the enrichment of iron-reducing bacteria. It is not yet known whether the iron reducers are responsible for its formation.

Lee plans to continue exploring the reductive dechlorination capability of the microbes from the extraction wells. It may be possible, some day, to use the microbes for remediation.

An internally-funded Laboratory Directed Research and Development (LDRD) project requiring the use of mesoscale reactors has been funded to monitor the effects of microbial growth (using the bacteria from the wells) on carbon tetrachloride transport in the vadose zone. Lee is conducting this project with INEEL researchers Bob Lenhard and Gill Geesey, in collaboration with Brigham Young University, the University of Stuttgart, and Pacific Northwest National Laboratory.

According to Mike Wright, director of the Subsurface Science Initiative, the key to making discoveries like Lee's is for scientists to continue to work with staff responsible for remediation, and vice versa. "This discovery is a good example of how cooperation is helping both research and remediation," Wright said. "I expect that as our understanding of the subsurface grows, discoveries of this nature will occur with greater and greater frequency, with the result that there will be more potential applications to solve DOE's problems."

Note: This research was funded by the INEEL Environmental Restoration Program and was conducted by Brady Lee.

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Organics Remediation in the Vadose Zone

The vadose zone beneath the INEEL's Subsurface Disposal Area contains volatile organic contaminants. These have migrated from the buried wastes in a vapor plume extending nearly 600 feet from the surface to the water table. Carbon tetrachloride is the greatest concern—sampling activities have revealed concentrations as high as 5,000 parts per million vapor (ppmv) of carbon tetrachloride in the plume.

A vapor vacuum extraction (VVE) process began remediating the vapor plume in Jan. 1996. As of Apr. 4, 2002, approximately 50,388 kilograms of volatile organic compounds have been removed and treated, including:

- 32,118 kilograms of carbon tetrachloride
- 7,563 kilograms of chloroform
- 7,071 kilograms of trichloroethane (TCE)
- 1,968 kilograms of 1,1,1- trichloroethane (TCA), and
- 1,668 kilograms of tetrachloroethylene (PCE).

Next Generation Vadose Zone Models

INEEL researchers are leading a three-year effort to improve groundwater modeling by incorporating mathematical complexity. In the process, they will test theories on the dynamics of flow in fractured rock systems. The project will create new algorithms that incorporate complexity through experimental observations of hydrological, geochemical, and biological factors influencing contaminant behavior.

> **"We're not out to prove that existing models are wrong, we're merely trying to improve them."**
>
> — Thomas Wood, INEEL hydrogeologist and principal investigator

The team, led by INEEL hydrogeologist Thomas Wood, believes that a shift in thinking is necessary to improve predictions of contaminant movement in the vadose zone. "We're not out to prove that existing models are wrong, we're merely trying to improve them," said Wood. (See box for discussion of determinism versus complexity.)

At issue are the discrepancies between deterministic predictions and the actual values of contaminant transport rates and concentrations that have been observed throughout the DOE complex. With determinism, explaining the discrepancies requires finding the source of error, either through questioning the characterization and monitoring data, or the models themselves—*something must be wrong*.

If the system is understood as complex in a mathematical sense, however, there is no expectation of knowing and predicting every detail of the system. "In a complex system, the sum of the parts is different than the whole," said Wood. "Deterministic models do not account for dynamic or emergent behavior, so they fail to recognize uncertainty for what it is."

> **"In a complex system, the sum of the parts is different than the whole. Deterministic models do not account for dynamic or emergent behavior, so they fail to recognize uncertainty for what it is."**
>
> — Thomas Wood, INEEL hydrogeologist and principal investigator

Wood uses the weather as an analogy to describe the need to better understand the vadose zone's complexity. "Even with detailed knowledge of all the factors—air and ocean temperature, moisture content,

(Next Generation continued on page 10)

Determinism versus Complexity

Determinism assumes that a system's state is an inevitable consequence of prior states and that the system itself is reducible. Similarly, stochastic approaches assume repeatable behavior resulting in statistically derivable probabilities for predictions. As a result, uncertainty in deterministic and stochastic models can always be decreased by refining input parameters for numerical simulations, increasing characterization and monitoring efforts, or increasing computational power.

Complexity, on the other hand, assumes that both reductive determinism and stochastic approaches are inadequate to capture the properties of a system. Complexity is not the property of having many parts (i.e., being complicated). Rather, it describes behaviors that are not reducible to one level of explanation.

To incorporate complexity, mathematical models must be built by approaching systems in new ways, not exclusively through traditional reductive methods. Models that incorporate complexity inherently accept that uncertainty cannot be eliminated.

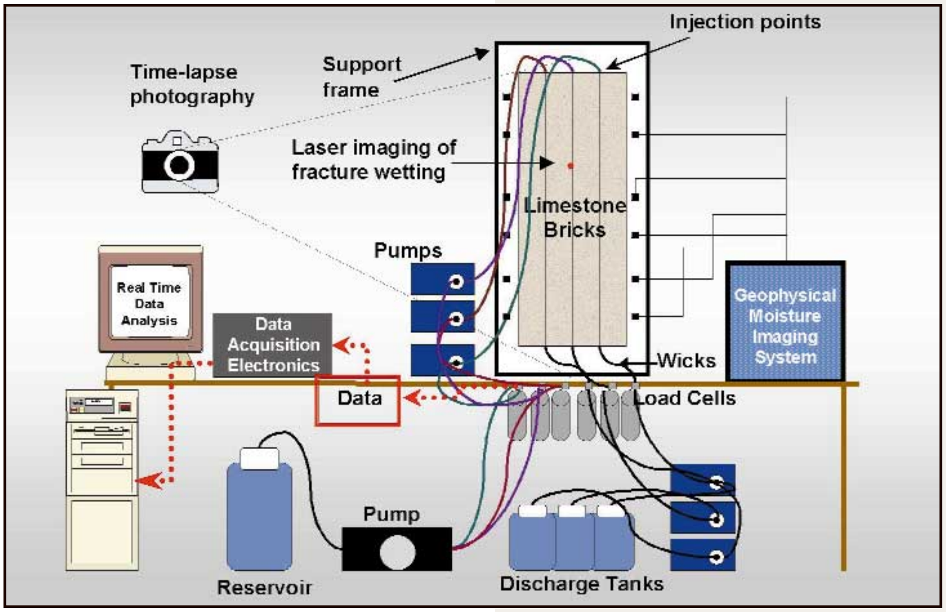


Figure 1. A schematic of the 12-brick system used in the initial experiments to observe flow paths through a fractured rock system.

(Next Generation continued from page 9)

air pressure, etc.—we understand and accept that weather is a complex and non-repeating system. Despite this, we have prospered by understanding general trends and patterns in the weather. Contaminant movement in the vadose zone is also complex, and can sometimes be unpredictable."

The hypothesis of complex behavior is being tested with a series of coupled, laboratory, mesoscale, small field-scale, and computer experiments. The first experiment was conducted in a simple fractured rock network—an uncemented brick wall of 12 limestone bricks standing on end, four bricks high by three bricks wide (see Figure 1). Water was dripped into the 'fractures' between the top bricks, and its flow path was observed. When the test was repeated, the flow path varied from that of the first test and continued to vary in subsequent tests.

Two important emergent properties were observed in this first experiment that are not accounted for in current vadose zone flow models. The first observation is that water accumulates at fracture intersections and then spurts onward, travelling more quickly and farther than expected based on the drip rate. This emergent dynamic is typical of complex behavior; small, sometimes imperceptible changes can precipitate sudden large reactions. Wood and his colleagues think that the fracture intersections work like small switches governing both the direction and the velocity of the flow. A small change in the switch's equilibrium causes sudden changes in the flow.

The second observation is that the water tends to converge at depth, collecting into a single flow path that travels much farther and faster through the rock network than expected. Even taking a broad array of variables into account, deterministic models failed to predict this effect.

The team decided its next step was to develop a better understanding of what happens in the fracture networks and what triggers the onset of complex behavior. This testing, which began with a simplified system of four limestone bricks, will expand in scope. A system with 24 limestone bricks—which is mounted to a weighing lysimeter—is currently being constructed.

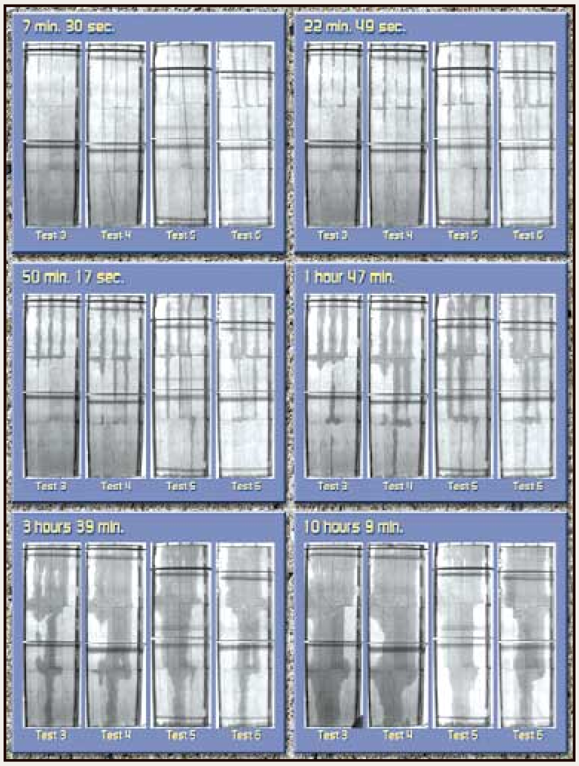
One of the main purposes of these experiments is to support the development of new algorithms that account for the chaotic behavior of vadose zone flow and transport. "Once we understand how each intersection acts in response to a wide range of parameters, we can develop a numeric model that incorporates this complex behavior into a fracture network with many intersections," said Wood.

Team member Randy LaViolette, a computational chemist at INEEL, is developing new mathematical approaches to process smaller time-series data sets that contain some level of noise generated by these experiments.

"Typically, patterns of complexity can't be discerned mathematically without huge amounts of clean time-series data," said LaViolette. "We are really pushing the limits mathematically. But it is important to develop an approach that supports the reality of the vadose zone."

Other models are also being studied for their application to flow dynamics and complexity. Team member and Sandia hydrologist Robert J. Glass has studied flow in single fractures for more than a decade. He is helping the team incorporate his work involving single fractures into larger fractured rock networks by advancing his *Modified Invasion Percolation Theory* approach to include dynamics created at fracture intersections. His approach is a type of

> ***" Predictions that are accurate in a general sense are more useful than predictions with overstated precision that prove to be inaccurate."***
>
> *— Thomas Wood, INEEL hydrogeologist and principal investigator*



Time-lapse photography of experimental runs in the 12-brick system (near right) shows significant variation in wetting patterns for tests conducted under nearly identical conditions. The patterns predicted using a conventional modeling approach (next page) fail to identify the variation and flow convergence observed in the experiment.

cellular automata—a method employed by other disciplines within the field of complexity.

David Peak, a Utah State University physicist, has been generating surrogate data sets using a self-organized dynamics approach. His results show remarkable similarity to the data sets collected by the INEEL researchers.

Ultimately, Wood's team expects that incorporating complexity will improve models by placing bounds on the possible outcomes, rather than attempting to predict movement in a deterministic way.

"Let's go back to the weather," said Wood. "It would be crazy to predict that the noon temperature on May 18 will be exactly 72°. By bracketing my guess—predicting it will be between 60° and 80°—I can make a reasonable prediction. Predictions that are accurate in a general sense are more useful than those with overstated precision that prove to be inaccurate. It's sufficient for raising crops and for predicting insult to the environment from contaminant migration."

Even though the team is far from developing new algorithms, two team members who work for the INEEL Environmental Restoration Program are already applying the new data analysis approaches for complex systems to groundwater data from the Radioactive Waste Management Complex.

In the future, experiments will apply the knowledge from the preliminary limestone experiments and introduce the variable of stimulated microbial growth. "Microorganisms also contribute to the complex dynamics observed in subsurface systems," said INEEL microbiologist Daphne Stoner.

Her experiments will monitor biofilm formation and flow rates to determine how microbial numbers affect fluid flow through fractured media. *Shewanella putrefaciens* cells, genetically tagged with green fluorescent protein, will be used. *S. putrefaciens* can live with or without oxygen, and plays a role in biogeochemical iron cycling, the natural attenuation of chlorinated solvents, and the fate and transport of radioactive materials in subsurface environments.

Eventually, the team will use basalt (native to INEEL) and begin conducting experiments in the field.

"If we are going to make better predictions, the current deterministic approach used for groundwater modeling needs to evolve," said Wood. "Our research is aimed at giving regulators and DOE more confidence in their predictions. That will be the big bonus."

Note: This research is funded by DOE's Environmental Systems Research and Analysis Program (ESRA) and is being conducted by: Thomas R. Wood; Daphne Stoner, Ph.D.; Randall LaViolette, Ph.D.; Robert C. Starr, Ph.D.; Molly Leecaster, Ph.D.; and Timothy McJunkin, Robert K. Podgorney, Karl Noah, and Thomas M. Stoops (all from the INEEL); Michael Nicholl, Ph.D. and Jerry Fairley, Ph.D. (UofI); Robert J. Glass, Ph.D. (Sandia National Laboratory); David Peak, Ph.D. (USU); and Douglas LaBrecque, Ph.D. (Multi-Phase Flow, LLC).

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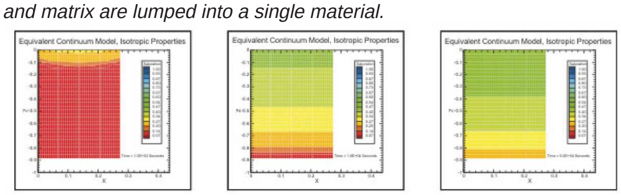
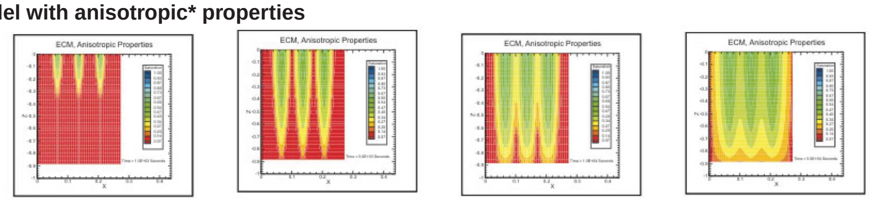
Conventional Modeling Results *(provided by Jerry Fairley, University of Idaho)*

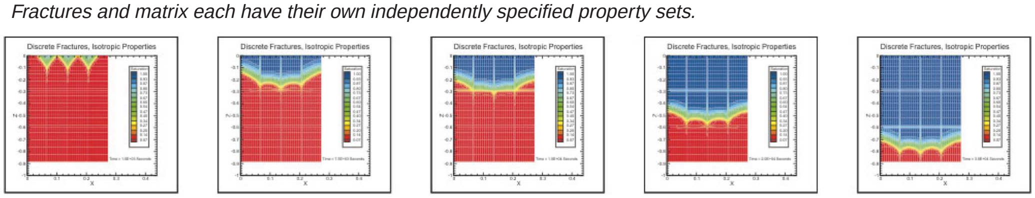
Equivalent continuum model (ECM) with isotropic* properties
The effects of fractures and matrix are lumped into a single material.



ECM model with anisotropic* properties



Discrete fracture model with isotropic* properties
Fractures and matrix each have their own independently specified property sets.



**Isotropic properties are the same when measured in any direction. Anisotropic properties vary depending on direction of measurement.*

INRA Doctorate in Subsurface Science Receives Funding

A new interdisciplinary and multi-institutional doctoral program in subsurface science will be offered through the Inland Northwest Research Alliance's (INRA's) Subsurface Science Research Institute (SSRI). The INRA Subsurface Science Graduate Program will allow students to develop understanding and expertise in several areas of study that are interrelated at the subsurface level, but have traditionally been studied in isolation.

The INRA graduate program will offer instruction in a variety of fields, such as biology, geology, hydrology, engineering, and geophysics, and is consistent with National Science Foundation (NSF) initiatives, such as the Integrative Graduate Education and Research Traineeship (IGERT) program, and also with recent recommendations for revising doctoral education in the United States.

The curriculum will incorporate the combined assets of the eight INRA universities and the specialized research infrastructure at the INEEL. Students will be able to take graduate-level courses from participating universities and interact with colleagues from other institutions as they work toward a Ph.D. degree.

"Each INRA institution has the opportunity to contribute its particular areas of expertise," said Gautam Pillay, INRA executive director. "Together, they are creating a common course curriculum that will offer a broader variety of courses for students at each of the INRA schools."

The program will be administered by a nine-member steering committee, consisting of the INRA executive director and the graduate deans from each of the INRA universities. Two support committees have already begun work—the Curriculum Development Committee (CDC) and the Instructional Design and Technology Committee (IDTC). The CDC is designing a curriculum that will take advantage of the best faculty in the different disciplines. The IDTC is working with the CDC to define a distance education technology that will deliver the curriculum to graduate students at the INRA campuses and at the INEEL.

"We anticipate that the students and future graduates of this program will be better prepared to undertake interdisciplinary research on subsurface processes and their numerous applications," said SSI director Mike Wright.

The INRA universities plan to enroll students in the fall semester of 2002. The universities include: University of Alaska-Fairbanks, Boise State, Idaho State, University of Idaho, Montana State, University of Montana, Utah State, and Washington State.

Note: The SSRI was created by an Energy and Water Appropriations Bill, which also provided $3.8 million in funding. The INEEL is funded in FY 2002 to participate in curriculum development.

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Call for Abstracts for Technical Posters for the 2002 Subsurface Science Symposium

The 2002 Subsurface Science Symposium, presented by INRA and the INEEL, will be held October 13-16 at the Doubletree Inn Riverside in Boise, Idaho. Although all subsurface science topics will be represented, the theme of this year's symposium is mesoscale research. For more information about the symposium, visit INRA's Web site at **www.inra.org**.

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